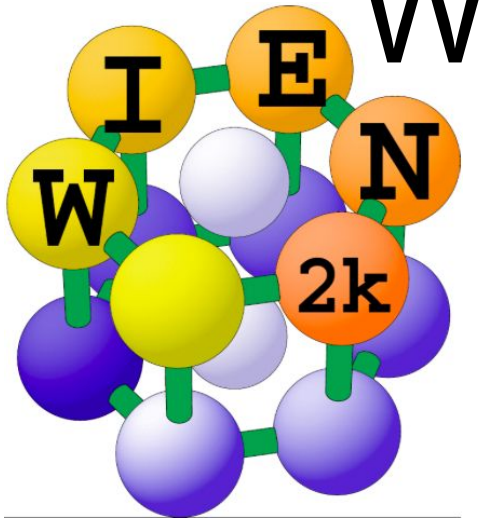

WIEN2k Tutorial

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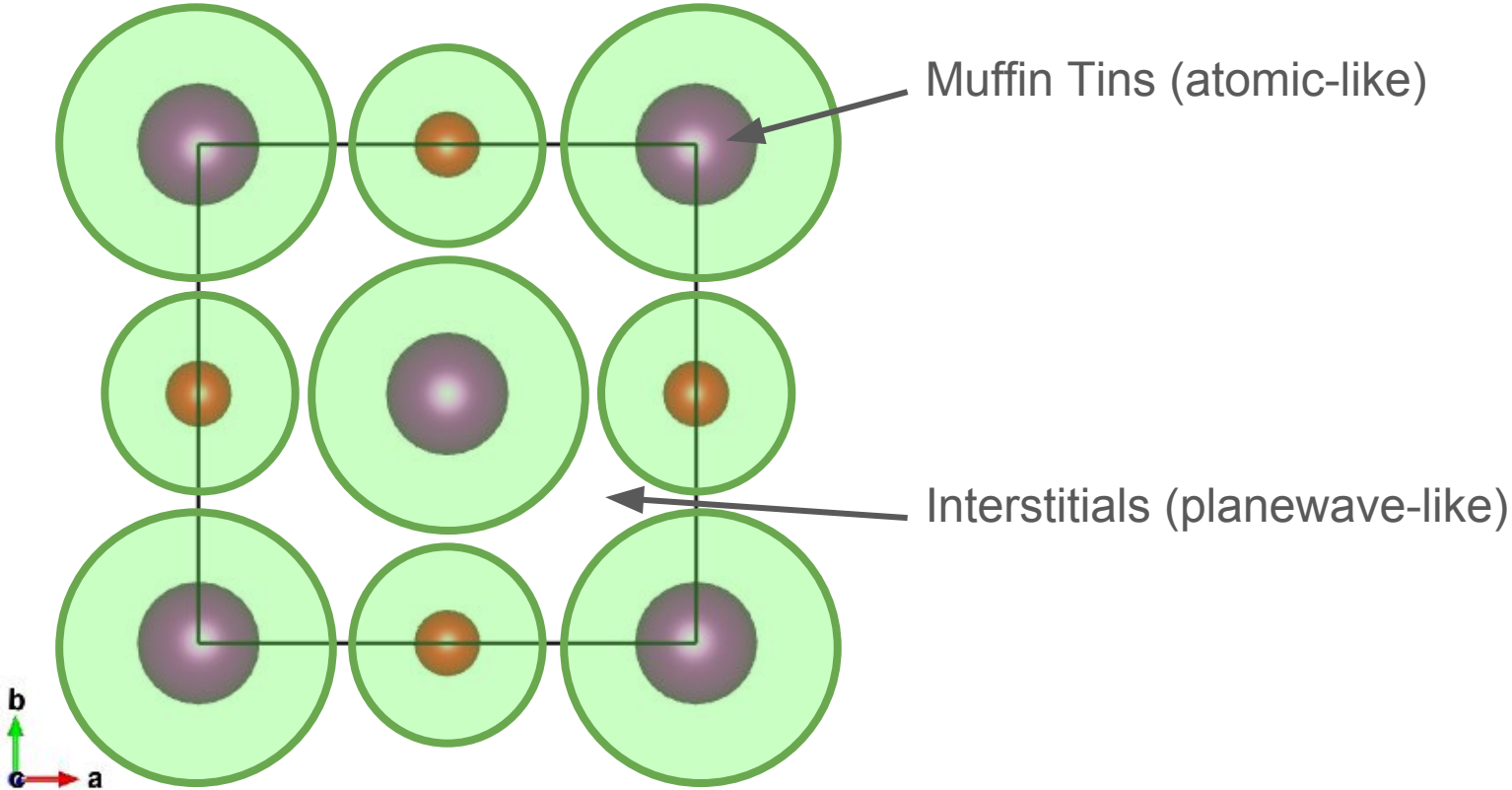
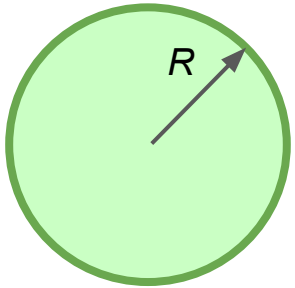
Wien2k Tutorial Outline

- Conceptual overview of APW+lo method
- Ex 1: MnO
- Introduction to Wien2k package and calculation workflow
- Key input and output files
- Ex 2: FeSe
- Ex 3: k-mesh convergence
- Ex 4: basis size convergence

Why do we need augmented plane waves (APW)?



Can we construct a basis well-matched to ψ?



$$e^{i\mathbf{q}\cdot\mathbf{r}}\big|_{r=R} = 4\pi \sum_{lm} i^l Y^*_{lm}(\hat{\mathbf{q}}) u_l(E,r) Y_{lm}(\hat{r}) \frac{j_l(qR)}{u_l(E,R)}$$

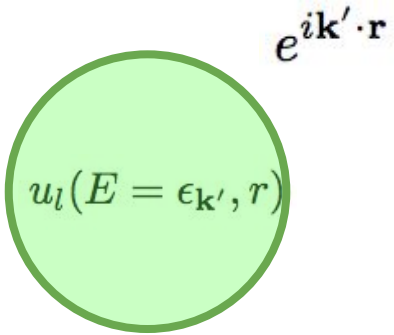
$$\phi_{\mathbf{q}}(E,\mathbf{r}) = \begin{cases} e^{i\mathbf{q}\cdot\mathbf{r}} & r > R \\ 4\pi \sum_{lm} i^l Y^*_{lm}(\hat{\mathbf{q}}) u_l(E,r) Y_{lm}(\hat{r}) \dfrac{j_l(qR)}{u_l(E,R)} & r < R \end{cases}$$

"Augmented plane waves"

How do we choose *E*?

Thought experiment:

$\mathbf{k}', \epsilon_{\mathbf{k}'}$



Choose:

$$E \sim \frac{1}{N}\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$$

Add additional orbitals inside sphere to capture variation missed by *E* = const

Called local orbitals (“lo”) ⇒ APW+lo

$$\phi_{\mathbf{q}}(\epsilon_{\mathbf{q}}, \mathbf{r}) = \begin{cases} e^{i\mathbf{q}\cdot\mathbf{r}} & r > R \\ 4\pi \sum_{lm} i^l Y^*_{lm}(\hat{\mathbf{q}}) u_l(\epsilon_{\mathbf{q}}, r) Y_{lm}(\hat{r}) \dfrac{j_l(qR)}{u_l(\epsilon_{\mathbf{q}}, R)} & r < R \end{cases}$$

Summary of APW+lo

Basis consists of:

1. Augmented plane waves (indexed by *k*)
2. Local orbitals (indexed by *lm*)

Alternative method for treating *k*-dependence of *E* via linearization

- “linearized” APW ⇒ LAPW
- Wien2k started out as LAPW code, evolved to APW+lo
- Still call *E* “linearization energy”, LAPW and APW+lo used interchangeably

For in-depth understanding: `http://www.wien2k.at/reg_user/textbooks/`

When to use APW+lo vs. planewaves?

LAPW / APW+lo

- Need high precision (esp. systems with partially-filled d or f shells)
- Smaller systems (< 50 atoms)

Planewaves:

- Larger systems and slabs
- Dynamical properties, e.g., phonons

What are the key numerical parameters?

1. XC potential
2. k-mesh
3. RKMAX
4. RMT
5. Ecut
6. Linearization energies

1. Exchange-correlation potential

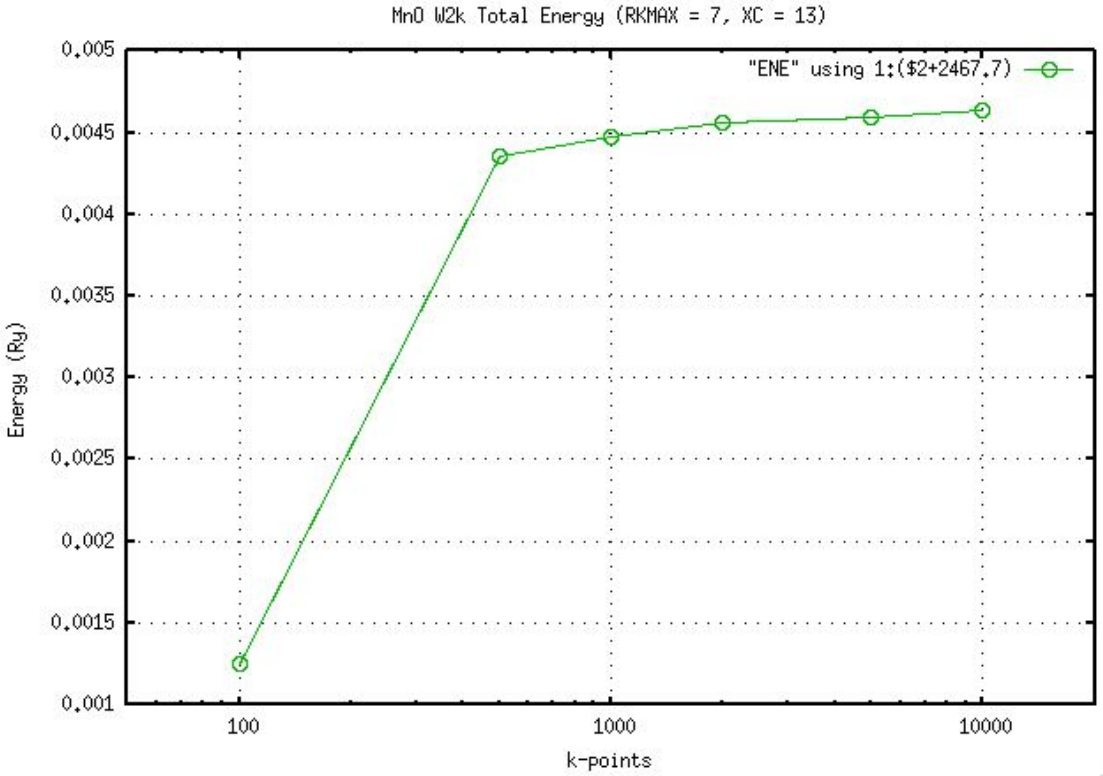
```
PBE    [(13) GGA of Perdew-Burke-Ernzerhof 96]

LDA    [( 5) Perdew-Wang parametrization of Ceperly-Alder data 92]

WC     [(11)  GGA of Wu-Cohen 2006]

PBESOL [(19) GGA of Perdew etal. 2008]
```

2. k-mesh: match to complexity & desired accuracy

In entire (reducible) BZ, need:

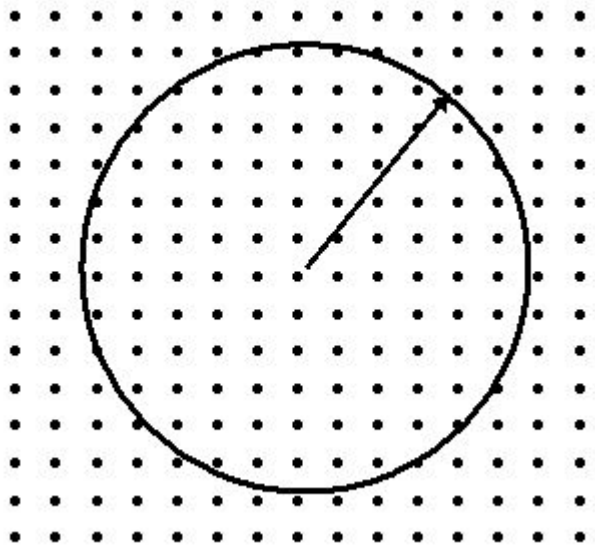
10-100kpts for insulators
or large unit cells

1000-10000 metals
or small unit cells

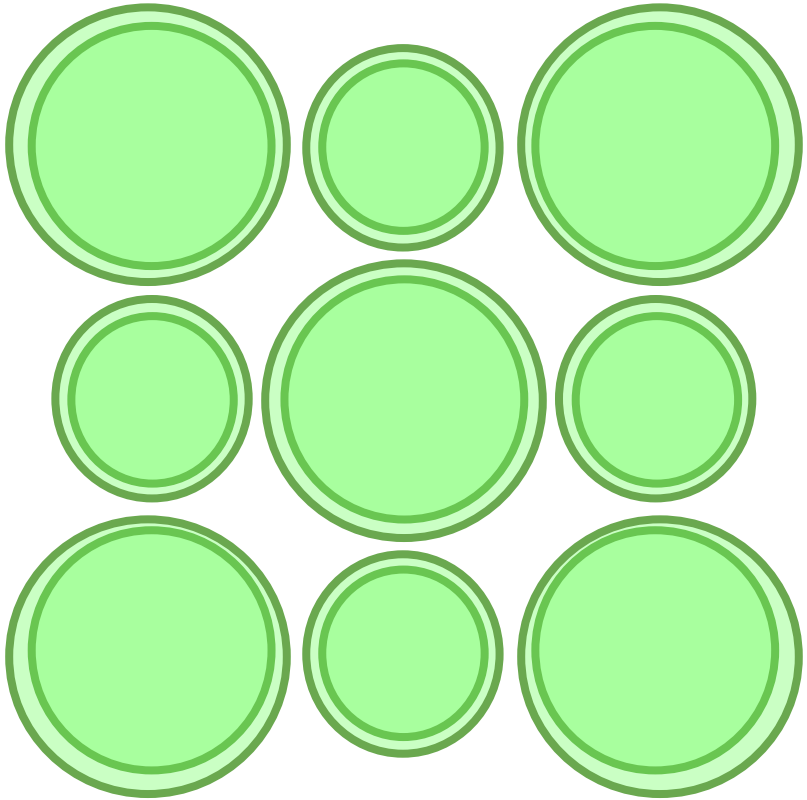


3. RKMAX controls basis size and accuracy

Planewaves: Kmax ~ accuracy



3. RKMAX controls basis size and accuracy



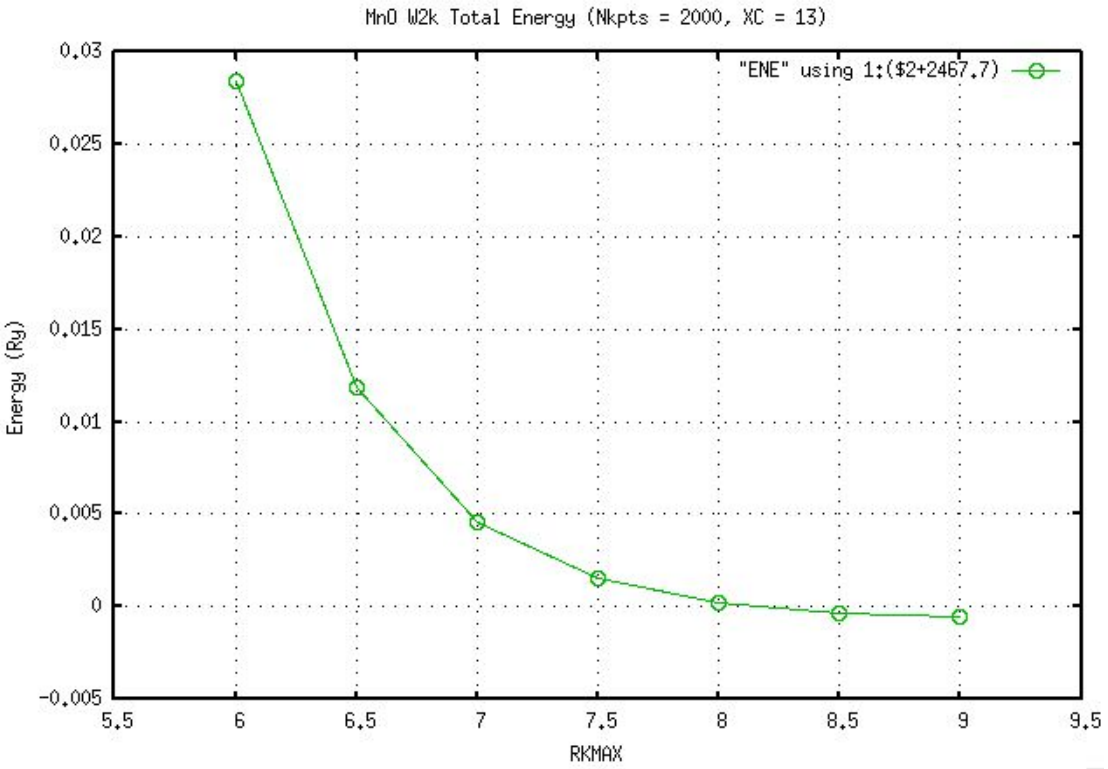
Planewaves: Kmax ~ accuracy

Rmin ↑ Kmax ↓

RKMAX = Rmin * Kmax

APW+lo: RKMAX ~ accuracy

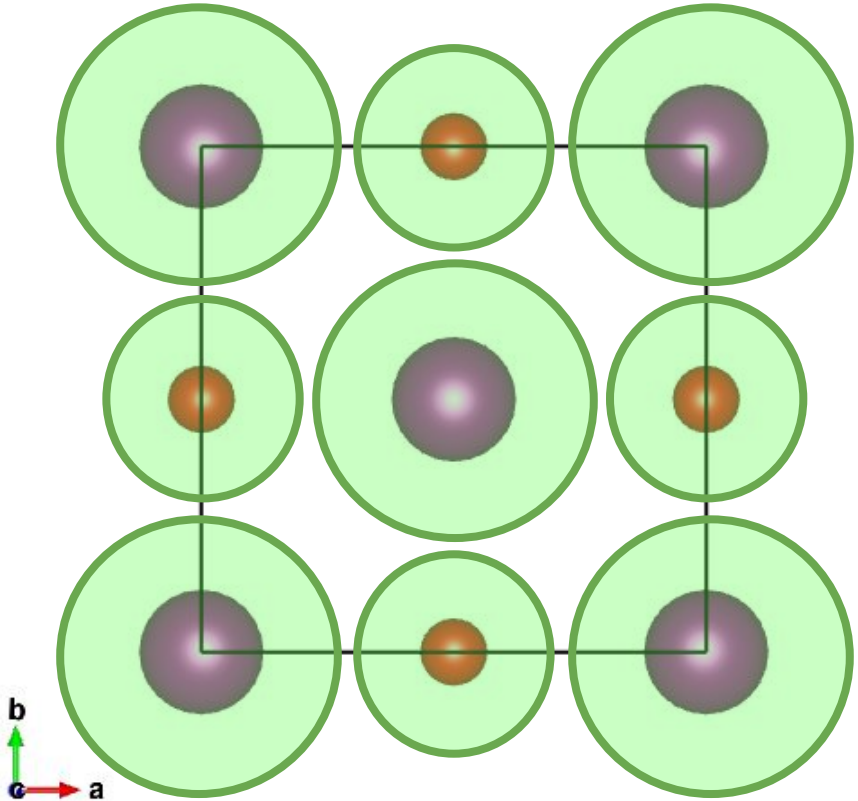
3. RKMAX: typical values range from 6-9



Wien2k default:

```
RKMAX = 7
```

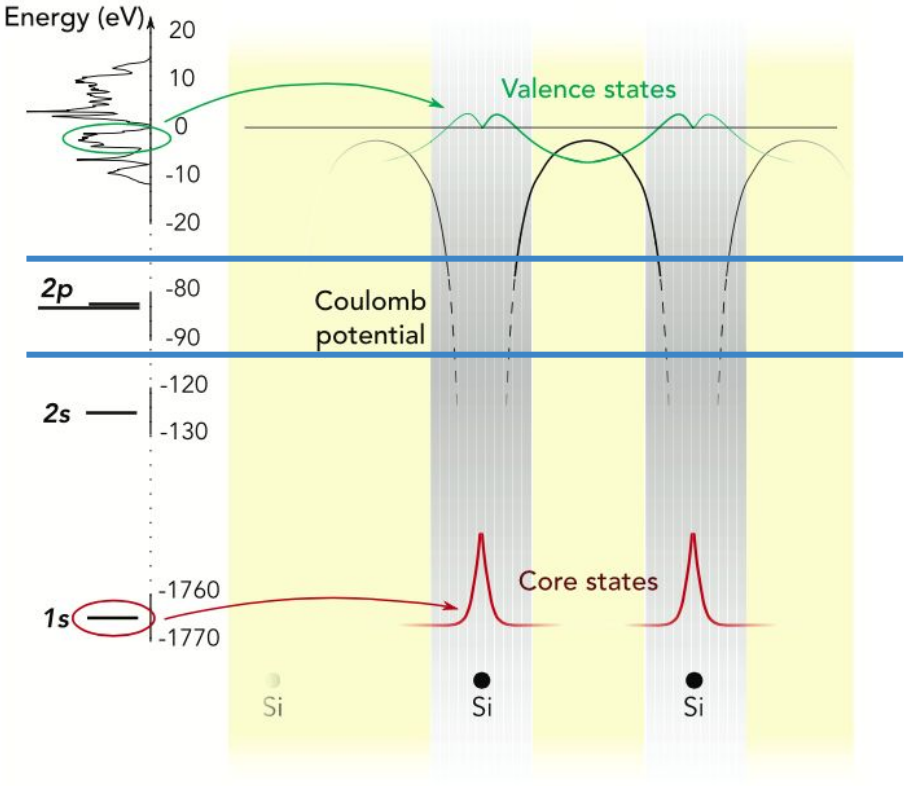
4. RMT ranges from 1.6 to 2.8 bohr



Roughly match “size” of atom.

As big as possible without touching.

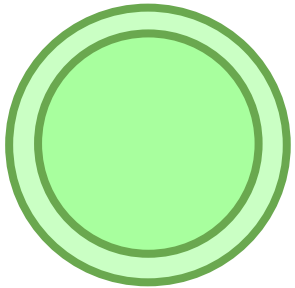
5. Ecut: choose to minimize core charge leakage



Bigger Rmin, smaller Ecut

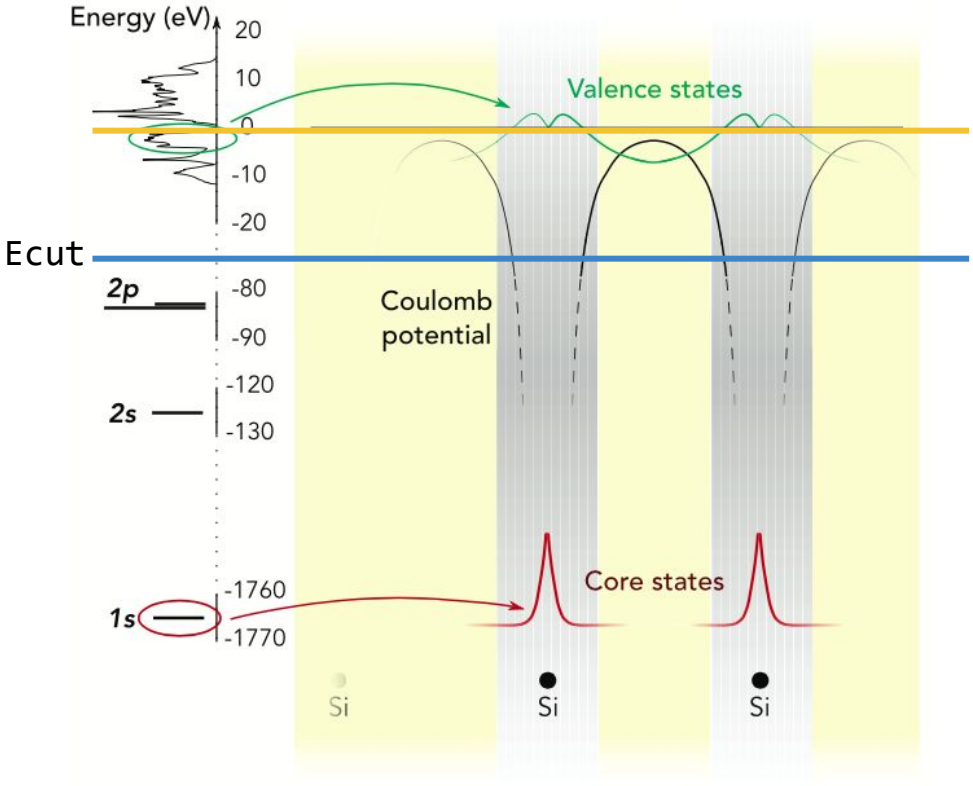
Wien2k default:

```
Ecut = -6.0 Ry
```



Science **351**, 1415 (2015)

6. Linearization energies



Choose close to center of band

Automatically chosen by Wien2k initialization

Often need to tune when using large RKMAX or have widely varying RMTs

Often a source of frustration for new LAPW / APW+lo users

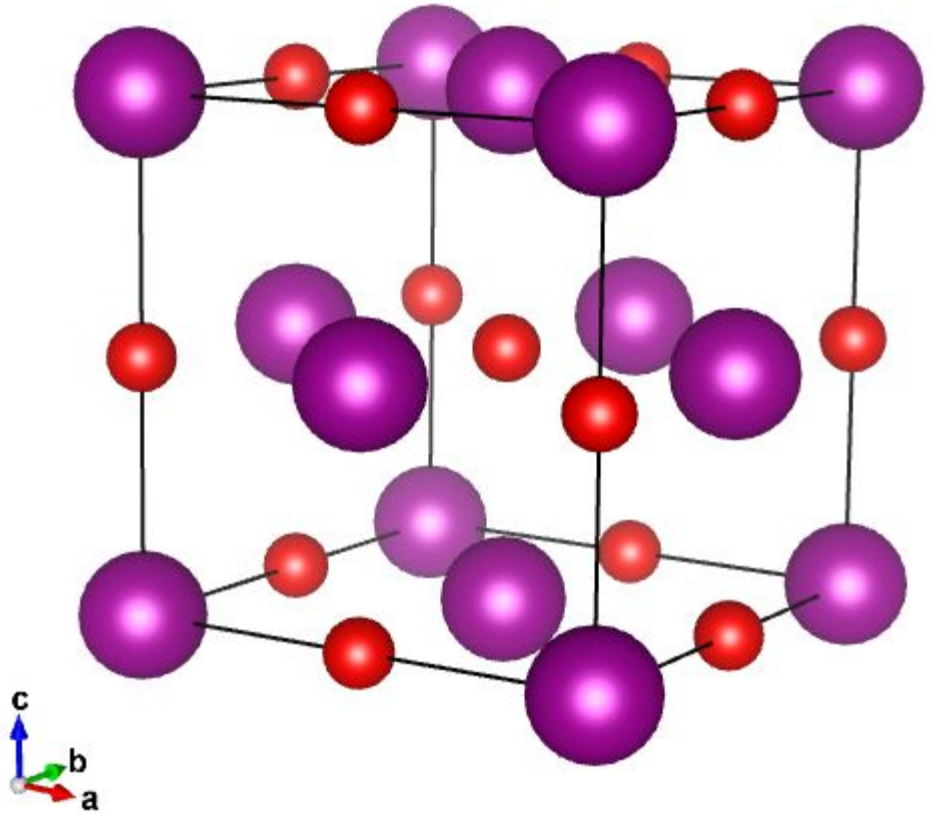
Science **351**, 1415 (2015)

Exercise 1: MnO

Simple rock salt structure

Mott insulator

Antiferromagnetic below 118K



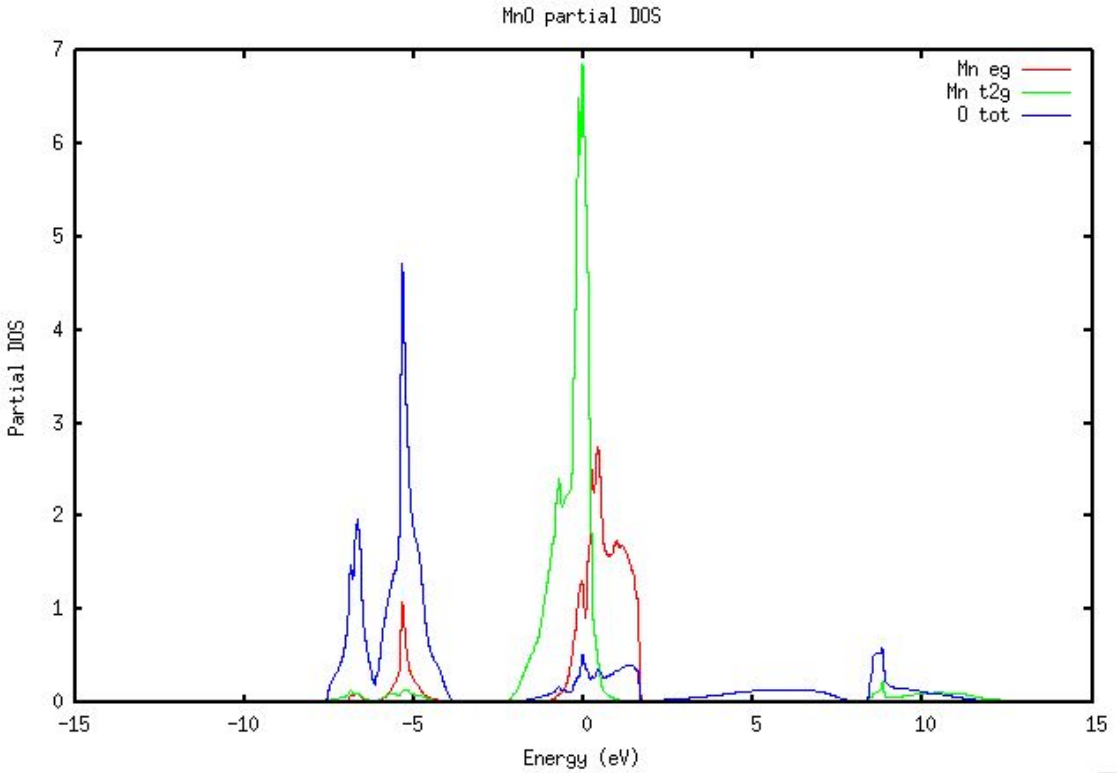
Exercise 1: Create the W2K inputs for MnO

```
$> ssh -X stud[..]@summer2016.ccs.usherbrooke.edu

$> qsub -I -X

$> module load edmftf

$> export OMP_NUM_THREADS=2

$> mkdir MnO; cd MnO

$> wget http://summer2016.ccs.usherbrooke.ca/w2k/MnO.struct

$> init_lapw -b -vxc 13 -ecut -6.0 -rkmax 7 -numk 500
```

Exercise 1: Run W2K and plot the MnO DOS

```
$> run_lapw

$> x qtl

$> wget http://summer2016.ccs.usherbrooke.ca/w2k/MnO.int

$> x tetra

$> wget http://summer2016.ccs.usherbrooke.ca/w2k/MnO.gnuplot

$> gnuplot -p MnO.gnuplot
```

Exercise 1: MnO density of states



Mainly Mn d states at Fermi level

Clear splitting between Mn eg (higher in energy) and t2g (lower in energy) densities

Oxygens below Fermi level

(Would need at least 10000 k-points for quality DOS)

Wien2k Package

Package composed of many Fortran90 executables linked by C-shell scripts

Two interfaces:

- Local web GUI (w2web)
- Console interface (batch and interactive)

Shell scripts have:

- Long names (`init_lapw, run_lapw, x_lapw`)
- Short names (`init, run, x`)

Creating a Wien2k run: naming and file conventions

Choose a unique name for each calculation, called “case”. Ex: `MnO`

Master input called “case.struct”. Ex: `MnO.struct`

Must be placed in a directory also named “case”. Ex: `~/MnO/`

All generated input/scf/output files have endings corresponding to program:

`MnO.in1, MnO.scf1, MnO.output1` ⇐ `lapw1`

SCF = self-consistent field (think: log files)

Wien2k Workflow

Calculation initialization: `init_lapw`

- Calls many F90 execs: `nn, sgroup, symmetry, lstart, kgen, dstart`

Calculation execution: `run_lapw`

- Calls F90 programs in SCF loop: `lapw0, lapw1, lapw2, lcore, mixer`
- Inter-process communication via filesystem

Analysis: many scripts executed via, e.g., `x qtl`

What are the key input files?

The `init_lapw` script generates ~50 files!

1. MnO.struct
2. MnO.in1
3. MnO.klist
4. MnO.int (for plotting on density of states)

1. MnO.struct: master struct file contains RMT

```
MnO_RT_SPG225_PRB_V1_PZ36_1970
F   LATTICE,NONEQUIV.ATOMS   2  225 Fm-3m
MODE OF CALC=RELA unit=bohr
  8.401155  8.401155  8.401155 90.000000 90.000000 90.000000
ATOM   1: X=0.00000000 Y=0.00000000 Z=0.00000000
          MULT= 1          ISPLIT= 2
Mn         NPT=  781  R0=.000050000 RMT= 2.24          Z:  25.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
ATOM   2: X=0.50000000 Y=0.50000000 Z=0.50000000
          MULT= 1          ISPLIT= 2
O          NPT=  781  R0=.000100000 RMT= 1.93          Z:   8.00000
LOCAL ROT MATRIX:    1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
  48      NUMBER OF SYMMETRY OPERATIONS
 1 0 0 0.00000000
 0-1 0 0.00000000
 0 0-1 0.00000000
       1
```

Refer to docs for details

2. MnO.in1: RKMAX and linearization energies

```
WFFIL  EF=.479755616725   (WFFIL, WFPRI, ENFIL, SUPWF)
 7       10    4 (R-MT*K-MAX; MAX L IN WF, V-NMT
  0.30    4  0      (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 1    0.30      0.000 CONT 1
 1   -3.79      0.001 STOP 1
 2    0.30      0.005 CONT 1
 0    0.30      0.000 CONT 1
  0.30    3  0      (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0   -1.55      0.002 CONT 1
 0    0.30      0.000 CONT 1
 1    0.30      0.000 CONT 1
K-VECTORS FROM UNIT:4   -9.0       1.5    21   emin / de (emax=Ef+de) / nband
```

3. MnO.klist: k-points and multiplicities in IBZ

```
         1          0          0          0          7  1.0 -7.0  1.5       500 k, div: (  7  7  7)
         2          1          1         -1          7  8.0
         3          2          2         -2          7  8.0
         4          3          3         -3          7  8.0
         5          2          0          0          7  6.0
         6          3          1         -1          7 24.0
         7          4          2         -2          7 24.0
         8          5          3         -3          7 24.0
         9          6          4         -4          7 24.0
        10          7          5         -5          7 12.0
        11          4          0          0          7  6.0
        12          5          1         -1          7 24.0
        13          6          2         -2          7 24.0
        14          7          3         -3          7 12.0
        15          6          0          0          7  6.0
        16          7          1         -1          7 12.0
        17          4          2          0          7 24.0
        18          5          3         -1          7 48.0
        19          6          2          0          7 24.0
        20          7          3         -1          7 24.0
END
```

4. MnO.int: specifies orbitals to produce DOS

Not generated by `init_lapw`. Need to create by hand or modify template.

```
Title
 -0.50 0.002 1.500 0.003  # EMIN, DE, EMAX, Gauss-broadening(>de)
  5    N   0.000          # NUMBER OF DOS-CASES below, G/L/B broadening (Ry)
    0    1   total        # atom, case=column in qtl-header, label
    1    1   Mn tot
    1    5   Mn d-eg
    1    6   Mn d-t2g
    2    1   O tot
SUM: 0 2                     # NUMBER OF SUMMATIONS, max-nr-of summands
2 5                       # this sums dos-cases 2+5 from the input above
```

What are the key output files?

Wien2k generates ~100 output files. Large files:

- MnO.clmsum -- charge density
- MnO.energy / MnO.vector -- band energies and eigenvectors

The key files we need to examine:

1. MnO.scf
2. MnO.qtl
3. MnO.dos1ev

1. MnO.scf: master output file

Key values tagged in lines beginning with colon. Values printed for each iteration.

```
:ENE -- total energy

:FER -- Fermi level

:QTLXXX -- partial densities inside sphere for XXXth atom
           (how many s, p, d, f electrons)

:BANXXXXX -- filling of XXXXXth band (metal vs. insulator)
```

1. MnO.scf: master output file

```
:ENE  : ********** TOTAL ENERGY IN Ry =         -2467.69564710
```

```
:FER  : F E R M I - ENERGY(TETRAH.M.)=   0.4795668223
```

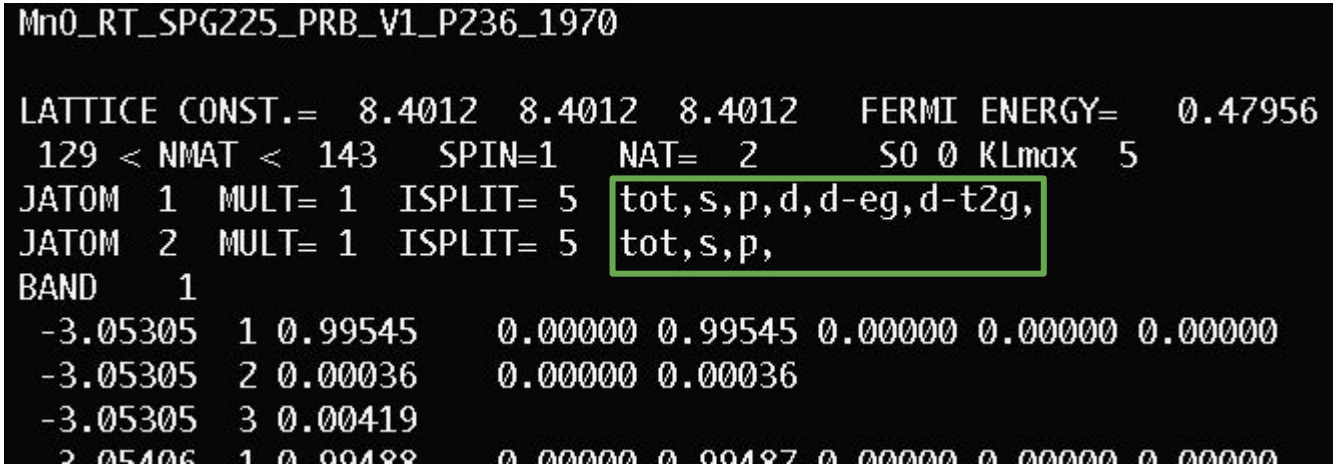
```
:CHA001: TOTAL VALENCE CHARGE INSIDE SPHERE   1 =  11.3166    (RMT=  2.2400 )
:PCS001: PARTIAL CHARGES SPHERE =  1 S,P,D,F,      D-EG,D-T2G
:QTL001: 0.1569 6.1414 4.9807 0.0300 0.0000 0.0000 0.0000 0.9381 4.0426 0.0000 0.0000 0.0000
```

1. MnO.scf: master output file

```
        Bandranges (emin - emax) and occupancy:
:BAN00002:   2   -3.056181   -3.053049  2.00000000
:BAN00003:   3   -3.054809   -3.053049  2.00000000
:BAN00004:   4   -1.004721   -0.934027  2.00000000
:BAN00005:   5   -0.076851    0.202734  2.00000000
:BAN00006:   6    0.026849    0.202734  2.00000000
:BAN00007:   7    0.079809    0.202734  2.00000000
:BAN00008:   8    0.313528    0.465826  2.00000000
:BAN00009:   9    0.396621    0.490394  1.85142990
:BAN00010:  10    0.396621    0.493787  0.97465673
:BAN00011:  11    0.438068    0.599999  0.14018201
:BAN00012:  12    0.438068    0.600503  0.03373136
:BAN00013:  13    0.505515    1.070919  0.00000000
:BAN00014:  14    1.095000    1.574030  0.00000000
:BAN00015:  15    1.134982    1.779019  0.00000000
:BAN00016:  16    1.419464    1.779019  0.00000000
:BAN00017:  17    1.550791    1.929864  0.00000000
```

2. MnO.qtl: orbital decomposition of bands

Generated by `x qtl`



3. MnO.dos1ev: density of states

Generated by `x tetra`. Partial densities selected in `MnO.int`

```
#  BAND   16
#EF=   0.00000     NDOS= 5     NENRG=  960    Gaussian bradening: 0.00300
# ENERGY  total-DOS        1:total         1:d-eg         1:d-t2g        2:total
 -13.32760    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.30039    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.27317    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.24596    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.21875    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.19154    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.16433    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.13712    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.10991    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
 -13.08270    0.00000000    0.00000000    0.00000000    0.00000000    0.00000000
```

How to obtain the master input file (case.struct)?

Crystallographic Interchange Format (CIF) is standard in community.

Can download CIF file from crystallographic databases, like ICSD or Materials Project.

Use utility `cif2struct` included with Wien2k to convert CIF to struct format.

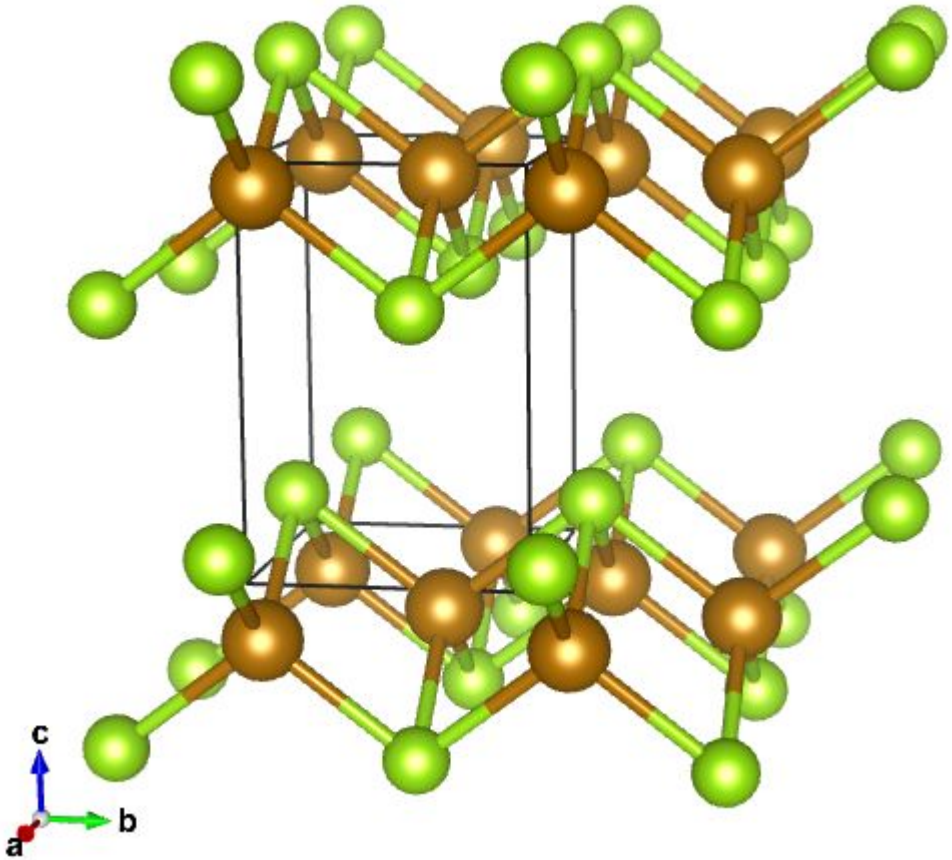
Exercise 2: FeSe

Iron-based superconductor

Tc = 9K to 37K (high-pressure)

Doesn’t require doping

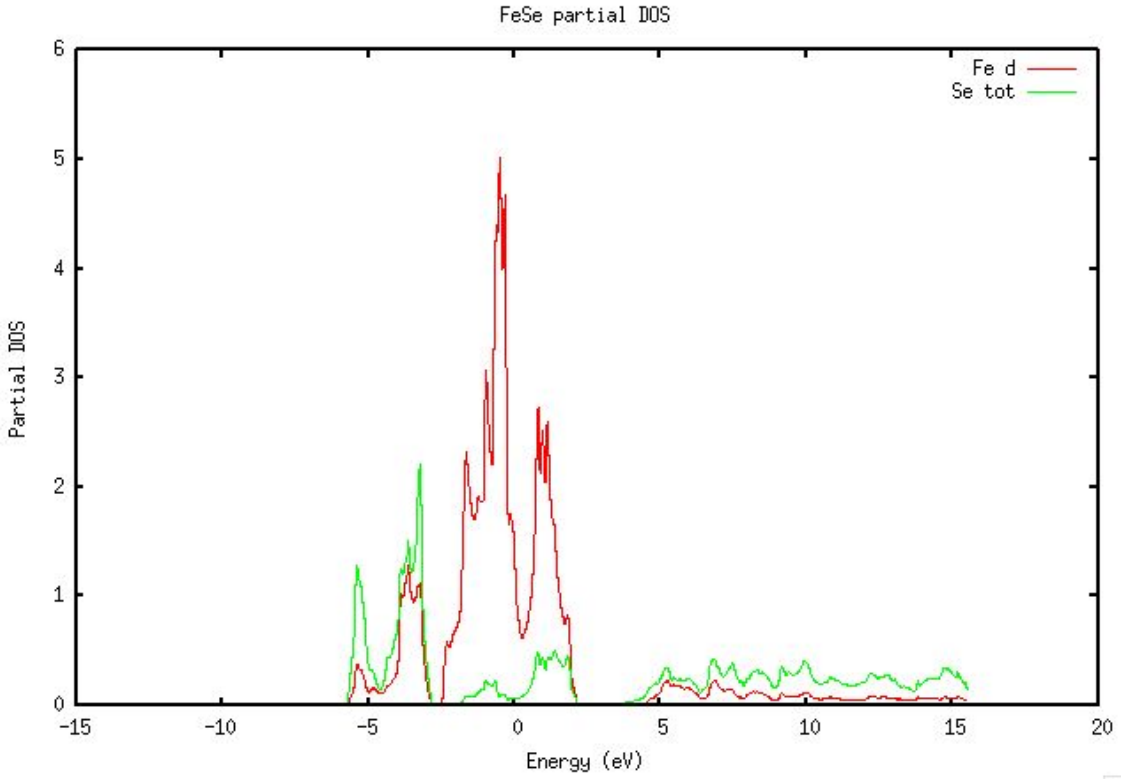
Heterostructures: possible superconductivity at ~100K



Exercise 2: FeSe -- run W2K and produce DOS

```
# create FeSe directory, get FeSe.struct, FeSe.int, FeSe.gnuplot
# from http://summer2016.ccs.usherbrooke.ca/w2k/

# initialize calculation; use the LDA (5) exchange-correlation
# potential and 500 k-points as before

# don’t forget to export OMP_NUM_THREADS=2

# run DFT, compute DOS and plot

# How would you edit FeSe.int to plot different partial densities?
#   (Docs at http://www.wien2k.at/reg_user/textbooks/)
```

Exercise 2: FeSe density of states



Fermi level composed mainly of Fe d states.

Se states below, strongly mixed with Fe states.

(Need many more k-points for high-quality DOS)

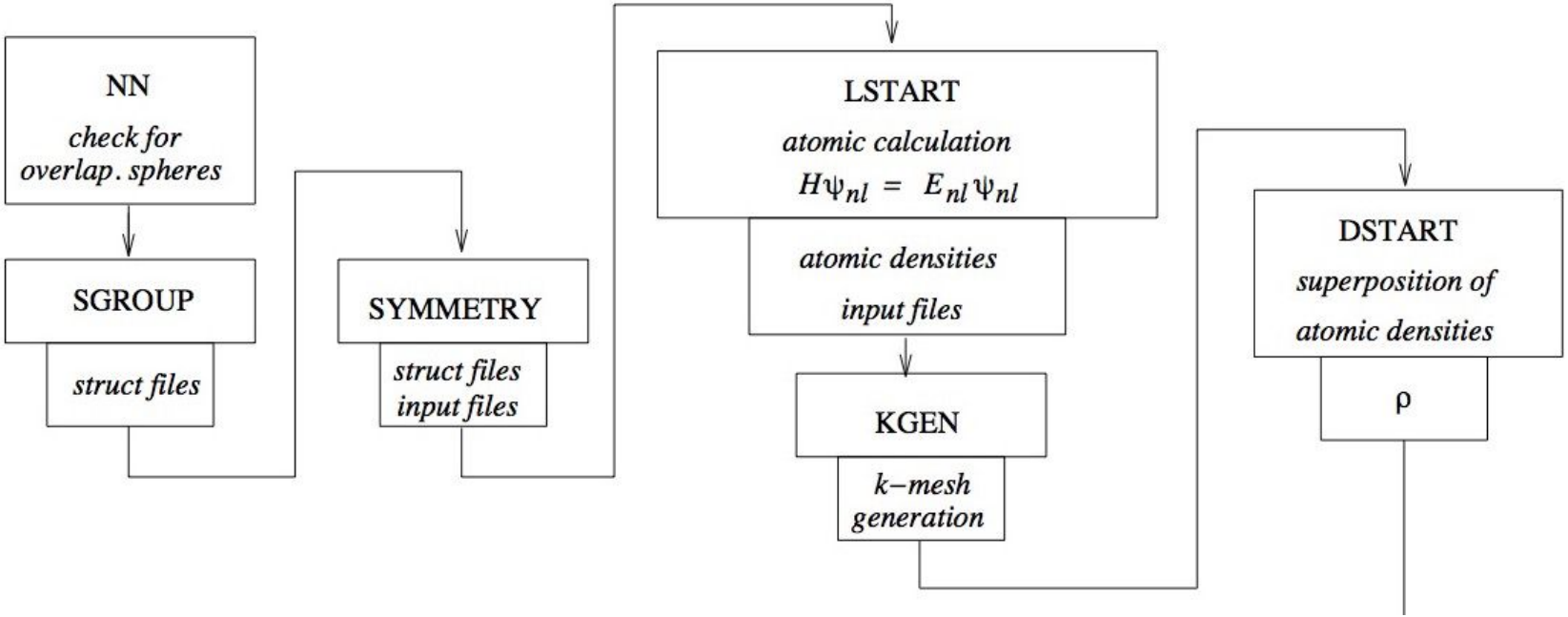
Exercise 3: MnO k-point convergence

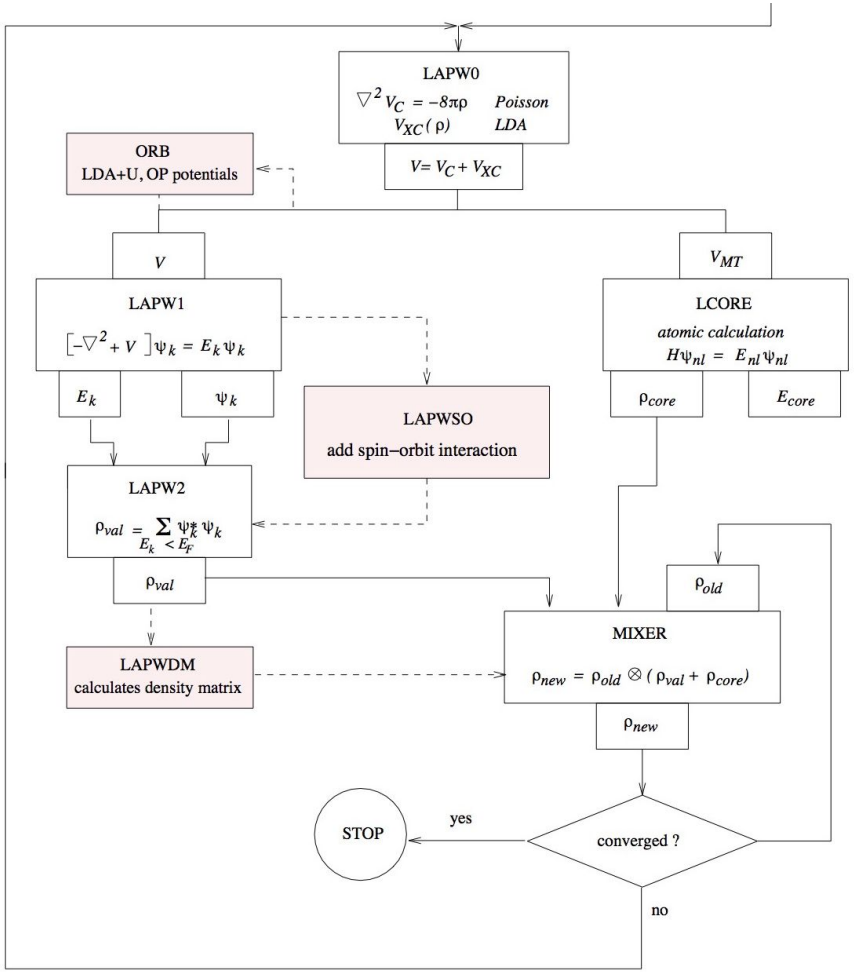
```
# Choose sequence of k-points to scan (100, 200, ..., 10000) and
# create corresponding directories (e.g. 100/MnO, 200/MnO, ...)

# Copy MnO.struct file into each directory, initialize
#   (recall the -numk flag for init_lapw) and run W2k

# The total energy at each iteration is printed in MnO.scf
#   (search for lines starting with tag ":ENE")

# Take the final energy (last one printed in MnO.scf) for each
# k-point run and plot (see figure on slide 10)
```

Exercise 4: MnO basis set convergence

```
# Scan RKMAX from 6.0 to 9.0 in steps of 0.5

# Setup directories, initialize files (use -rkmax flag) and run

# Again extract the final total energy (look for :ENE tag) for
# each run and plot against RKMAX (see figure on slide 13)
```

Supplementary Slides


NN
check for overlap. spheres
SGROUP
struct files
SYMMETRY
struct files
input files
LSTART
atomic calculation
$H\psi_{nl} = E_{nl}\psi_{nl}$
atomic densities
input files
KGEN
k−mesh generation
DSTART
superposition of atomic densities
ρ


LAPW0
$\nabla^2 V_C = -8\pi\rho$ Poisson
$V_{XC}(\rho)$ LDA
$V = V_C + V_{XC}$
ORB
LDA+U, OP potentials
V
V_{MT}
LAPW1
$[-\nabla^2 + V]\psi_k = E_k \psi_k$
E_k
ψ_k
LAPWSO
add spin–orbit interaction
LCORE
atomic calculation
$H\psi_{nl} = E_{nl}\psi_{nl}$
ρ_{core}
E_{core}
LAPW2
$\rho_{val} = \sum_{E_k < E_F} \psi_k^* \psi_k$
ρ_{val}
ρ_{old}
MIXER
$\rho_{new} = \rho_{old} \otimes (\rho_{val} + \rho_{core})$
LAPWDM
calculates density matrix
ρ_{new}
STOP
yes
converged ?
no

FeSe.struct master input file

```
FeSe structure
P                           2  129 P4/nmm
             RELA
  7.121433  7.121433 10.430154 90.000000 90.000000 90.000000
ATOM  -1: X=0.25000000 Y=0.75000000 Z=0.00000000
          MULT= 2          ISPLIT=-2
      -1: X=0.75000000 Y=0.25000000 Z=0.00000000
Fe  2+     NPT=  781  R0=0.00005000 RMT=    2.2400   Z:  26.00000
                    0.7071068-0.7071068 0.0000000
                    0.7071068 0.7071068 0.0000000
                    0.0000000 0.0000000 1.0000000
ATOM  -2: X=0.75000000 Y=0.75000000 Z=0.74000000
          MULT= 2          ISPLIT=-2
      -2: X=0.25000000 Y=0.25000000 Z=0.26000000
Se  2-     NPT=  781  R0=0.00005000 RMT=    2.1300   Z:  34.00000
                    1.0000000 0.0000000 0.0000000
                    0.0000000 1.0000000 0.0000000
                    0.0000000 0.0000000 1.0000000
  16       NUMBER OF SYMMETRY OPERATIONS
 1 0 0 0.00000000
 0 1 0 0.00000000
 0 0 1 0.00000000
       1
```

Bravais Lattice conventions

P	all primitive lattices except hexagonal	[a $\sin(\gamma')$ $\sin(\beta)$, a $\cos(\gamma')$ $\sin(\beta)$, (a $\cos(\beta)$)], [0, b $\sin(\alpha)$, b $\cos(\alpha)$], [0, 0, c]
F	face-centered	[a/2, b/2, 0], [a/2, 0, c/2], [0, b/2, c/2]
B	body-centered	[a/2, -b/2, c/2],[a/2, b/2, -c/2], [-a/2, b/2, c/2]
CXY	C-base-centered (orthorhombic only)	[a/2, -b/2, 0], [a/2, b/2, 0], [0, 0, c]
CYZ	A-base-centered (orthorhombic only)	[a, 0, 0], [0, -b/2, c/2], [0, b/2, c/2]
CXZ	B-base-centered (orthorh. and monoclinic symmetry)	[a $\sin(\gamma)/2$, a $\cos(\gamma)/2$, -c/2], [0, b, 0], [a $\sin(\gamma)/2$, a $\cos(\gamma)/2$, c/2]
R	rhombohedral	[a/$\sqrt{3}$/2, -a/2, c/3],[a/$\sqrt{3}$/2, a/2, c/3],[-a/$\sqrt{3}$, 0, c/3]
H	hexagonal	[$\sqrt{3}$a/2, -a/2, 0],[0, a, 0],[0, 0, c]

Local symmetry for orbital analysis

0	no split of l-like charge
1	p-z, (p-x, p-y) e.g.:hcp
2	e-g, t-2g of d-electrons e.g.:cubic
3	d-z2, (d-xy,d-x2y2), (d-xz,dyz) e.g.:hcp
4	combining option 1 and 3 e.g.:hcp
5	all d symmetries separate
6	all p symmetries separate
8	combining option 5 and 6
-2	d-z2, d-x2y2, d-xy, (d-xz,d-yz)

Local rotations for MnO vs. FeSe